**DICP-UCL Forum on Materials,**

**Catalysis and Energy**

**March 16th, 2013**

**Dalian, China**

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| **DICP-UCL Forum on Materials, Catalysis and Energy, 2013** | | | | |
| **Time Table of Forum Presentations (25min lecture, 5min discussion )** | | | | |
| **Date** | 16th March, 2013 | | **Place** | DICP, Biotechnology Building, Conference Room |
| **8:15-8:30 Opening Ceremony**  **Chair: Prof. Can Li** | | | | |
| 8:20-8:25 Welcoming Remarks Prof. Tao Zhang, Director of DICP | | | | |
| 8:25-8:30 Opening Speech Prof. Zhengxiao Guo, University College London | | | | |
| **Session One: Catalysts for Energy Conversion Chair: Prof. Zhengxiao Guo &Prof. Wenjie Shen** | | | | |
| 8:30-9:00 | | **Green and Controlled Synthesis of Nanoceramics for Energy/Catalysis Applications; From Lab to Pilot Plant Scale**  Prof. Jawwad Darr, *University College London* | | |
| 9:00-9:30 | | **Solar Hydrogen Production from Water by Heterogeneous Photocatalysis**  Prof. Fuxiang Zhang, *Dalian Institute of Chemical Physics, CAS* | | |
| 9:30-10:00 | | **CO2 Photoreduction to a Valuable Chemical or Fuel by Inorganic Photocatalysts**  Dr. Junwang Tang, *University College London* | | |
| 10:00-10:15 | | **Coffee Break** | | |
| **Session Two: Carbon Based Catalysts & Biomass Conversion Chair: Prof. Jawwad Darr & Prof. Hongxian Han** | | | | |
| 10:15-10:45 | | **Catalytic Transformation of Biomass to Ethylene Glycol**  Prof. Aiqin Wang, *Dalian Institute of Chemical Physics, CAS* | | |
| 10:45-11:15 | | **Synthesis and Characterisation of Carbon Nanostructures for H2/CO2 Sorption**  Dr. Congxiao Shang, *University of East Anglia* | | |
| 11:15-11:45 | | **Carbon for Catalysis**  Prof. Xiulian Pan, *Dalian Institute of Chemical Physics, CAS* | | |
| **Presentation from *Nature Communications*** | | | | |
| 11:45-12:15 | | **How to Get Published in *Nature Communications* (and its sister titles)**  Dr. Congcong Huang, *Nature Communication, China* | | |
| 12:15-13:15 | | **Lunch** | | |
| **Session Three: Nanomaterials for Catalysis Chair: Dr. Junwang Tang & Prof. Xiulian Pan** | | | | |
| 13:15-13:45 | | **Morphology-dependent Nanocatalysis: Rod-shaped Oxides**  Prof. Wenjie Shen, *Dalian Institute of Chemical Physics, CAS* | | |
| 13:45-14:15 | | **Nanostructured Materials for Catalytic Applications**  Prof. Gopinathan Sankar, *University College London* | | |
| 14:15-14:45 | | **“Oxide-on-metal” Inverse Catalysts for Low Temperature Oxidation Reactions: from Model Systems to Supported Nanocatalysts**  Prof. Qiang Fu, *Dalian Institute of Chemical Physics, CAS* | | |
| 14:45-15:00 | | **Coffee Break** | | |
| **Session Four: Energy Storage & Computational Study Chair: Prof. Gopinathan Sankar & Prof. Qiang Fu** | | | | |
| 15:00-15:30 | | **Design and Synthesis of Nanostructures for Energy Storage and Carbon Capture**  Prof. Zhengxiao Guo, *University College London* | | |
| 15:30-16:00 | | **Investigations on B-N Based Hydrogen Storage Materials**  Prof. Zhitao Xiong, *Dalian Institute of Chemical Physics, CAS* | | |
| 16:00-16:30 | | **Exploring Catalyst Support Materials in Fuel Cell Application with DFT Modelling**  Dr. Xin Xia, *Johnson Matthey Technology Center* | | |
| 16:30-17:00 | | **Kinetic Theory of Ostwald Ripening of Supported Metal Particles Under Reaction**  Prof. Wei-Xue Li, *Dalian Institute of Chemical Physics, CAS* | | |

**Prof. Gopinathan Sankar**

**[](http://www.google.co.uk/url?sa=i&rct=j&q=gopinathan+sankar&source=images&cd=&cad=rja&docid=koM4uF1TqcNfqM&tbnid=s1-kNDGuaTVO8M:&ved=0CAUQjRw&url=http://www.platinummetalsreview.com/article/55/4/233-245/&ei=SCotUf3rLsrV0QXK14DwDw&bvm=bv.42965579,d.d2k&psig=AFQjCNFJdApvmr5OwkRbGZ5a-Ctze60tXA&ust=1362000836775496)**

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Dr. Gopinathan Sankar is a Professor in the department of Chemistry, University College London, since 2007. He was educated in India. In 1990 he joined the Royal Institution of GB, London where he held several positions, including PDRA, Assistant Director of DFRL, Leverhulme Senior Research Fellow and Professor of Materials Chemistry. In 2007 he moved to Department of Chemistry, University College London as Professor of Solid-State Chemistry where he continues his research in the area of heterogeneous catalysis. His main area of research is heterogeneous catalysis with a focus on the study of nanoporous materials as multi-functional catalysts for a variety of reactions. Sankar’s group have developed in situ methods to follow crystallisation processes of a variety of catalytic materials, developed novel synthetic methods to produce catalytic materials, determine their structure in detail under operating conditions to correlate with catalytic properties. He specialises in the area of Synchrotron Radiation based X-ray techniques. Sankar was awarded a Royal Society Industry Fellowship and he closely work with scientists at Johnson Matthey in 2007. He has supervised over 25 PhD students and published over 200 papers in international scientific Journals. His current H-Index is 46.

**Nanostructured Materials for Catalytic Applications**

Gopinathan Sankar

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Catalysis is the back-bone of chemical industries and they will continue to be essential in numerous applications that are indispensable to enhance quality of our life and society. Several types of heterogeneous catalysts, for example, supported nano catalysts, nano-sized bulk oxides and nanoporous materials, are widely used for a variety of catalytic reactions. Within the family of heterogeneous catalytic systems, nanoporous and nano-sized systems are highly effective for performing selective catalytic reactions and hence studied widely for a variety of industrial applications. Although used widely there are several issues associated with the synthesis of these solids and more importantly designing the production of specific structures. Here in this presentation, novel synthetic methods of catalytic materials, in particular for designed synthesis of nano porous and nano-sized metal catalysts will be discussed. In addition, how in situ characterisation methods can provide detailed understanding to enable the development of synthesis strategy of the production of specific nano-sized materials will be discussed. Finally some catalytic applications in the area of plastic wastes to fuel, in situ generation of nano catalysts and application in the area of selective oxidation reactions will be discussed.

**Prof. Zhengxiao Guo**

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Zhengxiao Guo is a Professor of Materials Chemistry at UCL Chemistry and the London Centre for Nanotechnology. He is a guest professor of several renowned universities and research institutes in China. Xiao serves as a member of the editorial boards for several international journals. He was awarded the Beilby Medal 2000. He has been involved in and/or facilitated various UK-US, UK-Japan, UK-China and UK-Korea clean energy & nanotechnology links. He was also a UK representative of the Task 19 and then 22 of the International Energy Agency. He contributed to two MAT-UK’s energy strategic documents in 2007, launched by then DTI. He is now a Pro-Provost at UCL, the Focal-Point for UK-China collaborations in Nanotechnology & Materials Science (2009-2012). His scientific career builds on the development of experimental and theoretical approaches to tackling some of the most challenging issues in energy, environment and healthcare. He has contributed over 170 high-quality journal publications and 230 conference papers/presentations in the field.

Professor Guo’s research focuses on multiscale syntheses and simulations of nanostructures and materials for energy/hydrogen generation, storage, energy catalysis, biofuel cells and biointerfaces. Fundamental theories are coupled with *ab* initio, molecular dynamics, cellular automata and finite element simulations for materials design and discovery, while selected materials are synthesised by mechanochemical alloying, self-assembly, deposition and precipitation methods. Materials systems cover clusters, metals, hydrides, oxides, metal-doped carbon nanostructures, and functional hybrid systems that show desirable properties for clean energy and biomedical applications.

**Design and Synthesis of Nanostructures for Energy Storage and Carbon Capture**

Zheng-Xiao Guo

Department of Chemistry and London Centre for Nanotechnology,

University College London

Energy Storage and Carbon Capture are two key measures to reduce CO2 emissions and enable energy security. Storing and delivering energy carriers pose great scientific and practical challenges. New emphases on power smoothing in electricity grid and on energy supply from off-shore wind open up new opportunities for energy storage systems. Clear understanding of carrier interactions with host structures is essential to design efficient energy storage systems, particularly for H2 and Li+ ion for clean transport applications. CO2 activation has been a challenging issue in carbon capture. Fundamental simulations were employed to study the specific mechanisms of binding, activation and sorption of gaseous molecules in representative host structures for the design of efficient hydrogen/Li+ storage systems, as well as sorbents for CO2. Both experimental and theoretical approaches were applied to selected materials of high promise, including doped/defective carbon, doped hydrides, metal/amine complexes and stable electrode materials. Simulations have shown an exceptional capability of CO2 activation by metal doped carbon structures. Important avenues for further study are discussed to speed up the development of clean energy technologies.

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Professor Darr (JAD) works in sustainable manufacturing of nanomaterials, possessing unique world leading facilities for green nanoparticle production. JAD is an experienced inorganic materials chemist with over fifteen years’ experience working at the interface of supercritical fluids, (green chemistry) chemical engineering, nanomaterials syntheses and materials characterisation (88 publications/H index 20).

To date, JAD has been awarded > ca. £5.2 million of EPSRC and industrial funding as a PI or Co-I largely in clean technologies for production of a range of functional materials. With this substantive EPSRC (UK research council) support over the last decade, his group has developed continuous supercritical water flow reactors for manufacturing inorganic nanomaterials; this has now been developed for scale-up pilot production of nanomaterials on kg/h scale at UCL. This process has many advantages as it overcomes batch processes which are variable and also it uses supercritical water (a green solvent). Much of his recent research has been in collaborations for the development of nanomaterials for energy storage, energy conversion, photocatalysis, CO2 reduction catalysts, biomedicine, security, pigments, catalysts, etc. JAD, is currently the UCL MAPS (Maths and Physical Sciences) faculty knowledge transfer champion with an agenda to support fellow academics in better interacting with industry. He is LTN network fellow (now alumni) and has also interacted very strongly with UCL Business.

**Green and Controlled Synthesis of Nanoceramics for Energy/Catalysis Applications; From Lab to Pilot Plant Scale**

Jawwad Darr

*Department of Chemistry, University College London*

Clean Materials Technology (CMT) at University College London has developed a range of nanoparticle metal oxides and metals (length scales 10 - 100 nm) produced using a state-of-the-art suite of continuous hydrothermal flow synthesis (CHFS) platforms. These platforms include laboratory-scale (200g/h) CHFS reactors and custom high throughput CHFS platform for rapidly producing large numbers of different types of nanoparticles. A pilot plant CHFS reactor has also now been developed to investigate scale-up of nanoceramics (> x5 times over current lab scale process); this plant can make up to 1kg /h (dry weight) of nanoceramics in a water based dispersion. Products from CHFS are in the form of an aqueous dispersion, avoiding hazards of airborne nanoparticles. Many different types of nanoceramic oxide particles have been produced for a wide range of ceramics applications (typically with surface areas from 200-400 m2g-1). Importantly, the nanoparticles can be readily given surface functionality, either in- or ex-process such for use in energy or catalysis applications. Professor Darr will outline these technologies as well as some of the issues relating to potential commercialization of the CHFS pilot plant for the production of high value nanoceramics for industry.

**Dr. Junwang Tang**

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Dr Tang is a Senior Lecturer/Associate Professor in Energy in Chemical Engineering at University College London (UCL) and an Honorary Lecturer in Chemistry at Imperial College. He has been focusing on nanocrytalline materials and nanostructured films fabrication and their application in renewable energy production and environmental purification (gas and liquid phase) since 1995. Currently, his research interests lie in i) solar energy conversion to fuels, including solar H2 production by water photolysis and CO2 conversion, ii) hybrid solar cell, iii) organic contaminant photo-mineralisation and iv) Microwave assisted microfluidic system for nanomaterial engineering. In detail, his research goal is to utilise the diverse advanced technologies to prepare size and morphology-controlled materials and in-situ grow films on different substrates. Further the prepared porous, robust and nanostructured particles (including junctions) and films can be employed either to harness solar energy to generate fuels (e.g.: hydrogen, alcohols etc.), electricity or decompose contaminants in collaboration with other scientists in EU and outside. Such studies are undertaken in parallel with functional characterisation, mechanistic observation and device optimisation to address renewable and clean energy generation and eliminate GHG emission etc.

He currently leads a research team of 17 members addressing these topics, with financial support from UK EPSRC, Leverhulme, RS, RAE, EU PF7 and Qatar. He sits on the editorial board of several international journals. He is also the Vice President of the Chinese Society of Chemical Science and Technology in the UK, the Facilitator of Energy Research between UCL and Chinese Academy of Sciences and Champion of Solar Energy in the UCL CO2 Technology Center.

**CO2 Photoreduction to a Valuable Chemical or Fuel by Inorganic Photocatalysts**

Junwang Tang

*Department of Chemical Engineering, University College London*

Of all renewable energy sources, solar energy is the most abundant in the world. It has the potential to meet the increasing global energy demand. However achieving this potential requires significant technological advances. Therefore there is significant interest in efficient solar fuel synthesis by inorganic low cost photocatalysts (Artificial leaf concept). (1)

Among the approaches of solar energy conversion and storage, CO2 conversion to valuable chemicals and renewable energy by sunlight, characaterised by clean energy supply and CO2 emission reduction, has been attracting more and more interest over the last several years after a long-term silence. However to achieve stoichiometric CO2 reduction using water as a donor is still a big challenge because both reactions are multi-electrons/holes processes, kinetically being very difficult.(2) Therefore there are few reports on stoichiometric CO2 photoreduction and water oxidation by an inorganic photocatalyst in a heterogeneous system in the absence of bias and/or sacrificial reagents. In this talk, I will present recent results on CO2 photoreduction in my group by inorganic photocatalysts to illustrate the feasibility of CO2 photoreduction using water as electron donor in the absence of a bias or sacrificial reagent. Further, we study the feasibility of using Cu2O and Cu2O-based junction materials for photocatalytic CO2 reduction under visible light. It has been found that the junction structure dramatically increases the lifetime of electrons in Cu2O, resulting into nearly 7 times higher activity compared with pure Cu2O.

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Congxiao is currently a lecturer in energy materials and technology in the School of Environmental Sciences, University of East Anglia (UEA). Her research is focused on experimental development of high-surface area / porous nanostructures for clean energy technologies, including: 1) hydrogen storage/purification for clean transport vehicles; 2) CO2 capture for clean power generation; and 3) effective sorbents for pollutant removal and gas separation. The research activities are in close collaboration with scientists and industrialists nationally and internationally, e.g. at UCL/London, GasPlas/Norwich, Norner and Sintef/Norway, and Xiamen University/China. Her research has been sustained by a steady flow of research grants from the research council (EPSRC), the Royal Society, and industry in collaboration with a regional SME, GasPlas Ltd. as a partner of a £2m grant by Norwegian Science Research Council. By means of thermal, mechanical and chemical methods, she has synthesised Mg-based hydrogen storage materials that effectively halve the desorption temperature. With a novel microwave cold-plasma reactor and a magnetron sputtering system (PVD), she has developed high-surface area carbon nanostructures, which largely enhanced gas sorption / separation and can potentially enhance energy density as battery electrode. Her Research achievements were recognised by high-impact outputs in journal publications, invited national and international meetings and presentations.

**Synthesis and Characterisation of Carbon Nanostructures for H2/CO2 Sorption**

Congxiao Shang

*School of Environmental Sciences, University of East Anglia*

Our research investigates the chemisorptions and physisorption processes using chemisorbent metals and physisorbent structures, thus harnessing the best features of both materials to generate suitable adsorbents [1, 2]. Nanostructured carbon was produced by methane cracking in a relatively low-energy cold plasma reactor designed in-house [3]. The structures of carbon are examined by BET surface area, pore-size distribution, XRD and TEM. Carbon samples collected at different positions in the reactor show similar structural morphologies, indicating extensive structural uniformity of the carbon during processing. The variations in BET surface area and pore volume of the carbon materials are closely associated with the magnitude of temperature drop at the sample collection position in the cold-plasma chamber before and after methane loading. Further modifications of the carbon structure to enhance the surface area were carried out in a thermal furnace. An overview of recent results will be presented including the effects of carbon structures on hydrogen sorption of catalysed MgH­2 [4].

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Dr Xin Xia obtained his PhD in 2010 from the University College London (UCL). He received his MEng from Queen Mary, University of London, and his BSc form Beijing University of Aeronautics and Astronautics (BUAA). He is currently a research scientist in core science group of Johnson Matthey Technology Centre, UK (2011 to current).

His research interests include: catalyst and catalysis reactions, clean energy materials and computational modelling approaches of material selection and design. He also worked as a senior engineer of Lithium battery research at Amperex Technology Limited, China.

**Exploring Catalyst Support Materials in Fuel Cell Application with DFT Modelling**

Xin Xia

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Fuel cell technology offers an attractive combination of highly efficient fuel utilisation and environmentally friendly operation. In low temperature fuel cells, such as PEMFC, the electrochemical reaction must occur at a sufficient rate to give electrical output. This is achieved by using Platinum/precious metal based catalysts. Due to the scarcity and high cost of precious metals, the catalyst support which provides a physical surface for Pt distribution emerges as an important area of research to improve the mass activity of the metal catalyst. Currently, carbon is a common choice for supporting nanosized electrocatalyst particles. However, the conductive carbon support is susceptible to corrosion due to the harsh operating conditions in the fuel cell. Also, at high loading on carbon, Pt and other precious metal catalysts tend to form large nanoparticles with intrinsically low dispersions. Neither the carbon support nor the highly dispersed particles are sufficiently stable in the fuel cell environment. Various alternatives to carbon as electrocatalyst supports have been studied in the literature. In this study, we screened different types of catalyst supports using a computational approach. The influences of support materials have been studied in terms of geometric and electronic effects. The support-catalyst interactions, the desired properties of support stability, Pt wettability and catalytic activity have been investigated through DFT modelling.



**Dr. Congcong Huang**

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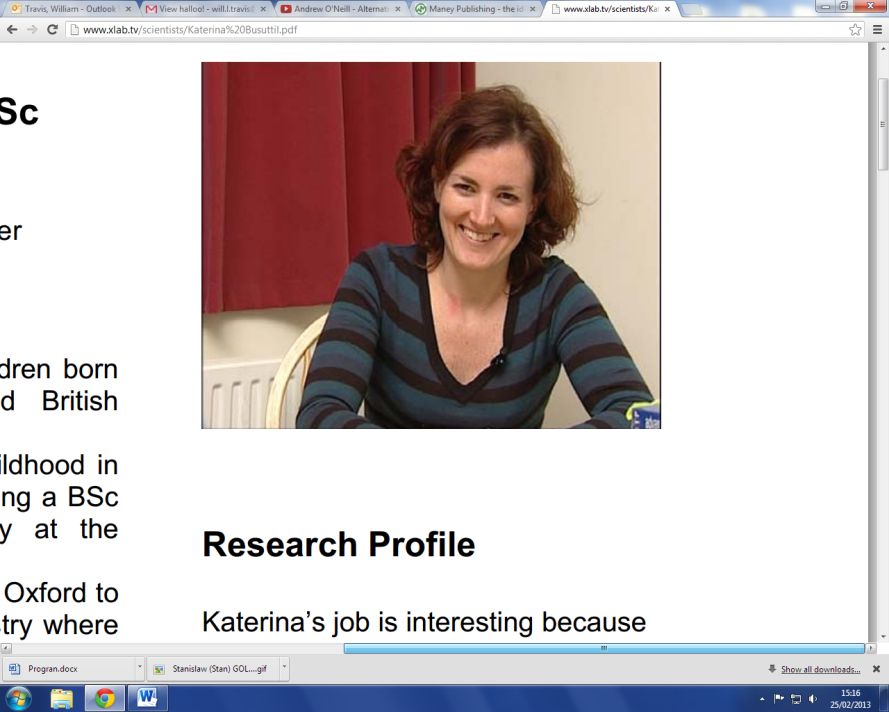
Congcong became a member of the Nature Communications team in June 2012. A graduate of Peking University in China, Congcong obtained a PhD in physics from the University of Cambridge in 2006, where she majored in surface physics. Congcong's subsequent postdoctoral research at Stanford University and SLAC National Accelerator Laboratory focused on hydrogen-bonded liquid structures using various synchrotron-based X-ray techniques and free-electron lasers. Her research interests also include amorphous materials, critical phenomena and coherent diffractive imaging.

**How to get published in *Nature Communications* (and its sister titles)**

Dr. Congcong Huang

*Associate Editor, China, Nature Communications*

So, you've discovered something extraordinary and you want to tell the world about it. Why would you publish it in a Nature journal? Which one should you choose? Indeed, why has Nature spawned so many new titles? What is *Nature Communications*, and what is it trying to do that other Nature journal don't do already? What is Open Access? In this talk I'll try to answer these and any other questions you have about getting published in a Nature journal. I'll also cover: what we look for in the papers that we consider for publication; the mechanics of how submissions are handled; how to decide if your paper could be for us; how to prepare a submission; and what to do when you think we (or our referees) have got a decision wrong. And, of course, what are we looking for in China?

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Dr Busuttil obtained a BSc in Chemistry and Biology at the University of Malta. Following that she went to Oxford to read for a D. Phil in chemistry where she worked on atomic force microscopy and nanotechnology. After some more time working in the lab, she took on her job working for Elsevier and AIP, then 2 postdocs, and now works for Maney who publishes Institute of Materials Journals.



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Mr. Travis is a PhD researcher working as part of the Zheng Xiao Guo group in the Department of Chemistry at the University College London (UCL). He received a Master’s in Chemistry from the University of Manchester focusing on organic synthesis. Currently his research interests lie in i) the development of novel porous materials, achieved through the development of porous polymers using rigid linking groups and also through controlled carbonisation of selected polymers, ii) the development of functionality within porous materials, in particular nitrogen content of different types, iii)N-doped porous materials derived from graphene oxide. The main focus for applications is gas storage, in particular hydrogen, methane and carbon dioxide.

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Mr Kaipei is a first year PhD student working in Prof. Zheng Xiao Guo’s group in the Department of Chemistry at the University College London (UCL). He received a dual BSc. Degrees in Environmental Science from Fudan University and University of East Anglia (UEA). He used to study in Dr. Congxiao Shang’s group as an undergraduate project student working on hydrogen storage materials (magnesium hydride) and now his research interest is electrochemical energy storage, particularly zinc-based flow batteries for grid-scale application. His current project is to find efficient metal-free catalysts (i.e. nitrogen-doped porous carbon) for oxygen reduction reaction (ORR), facilitating the development of high-capacity zinc-air batteries.

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Tao Zhang received his PhD in physical chemistry from Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences, in 1989 under the supervision of Prof. Liwu Lin. After graduation, he worked as a postdoc with Prof. Frank Berry at Birmingham University for one year. He founded his own group at Dalian Institute of Chemical Physics in 1995. He was appointed as an associated professor in 1993 and then promoted to full professor in 1995. Dr. Zhang has also been an invited professor at Univesity of Poitiers (France) in the period of 2006-2007 and a guest professor at University of Namur (Belgium) since 2011. Dr. Zhang is the director of DICP (since 2007) and the director representing the China aside of the China-France Joint laboratory for Sustainable Energy (since 2008).

Over the past decades, Prof. Zhang has successfully designed a great number of nano and subnano metallic catalysts for applications in energy conversion (such as biomass catalytic conversion and propellant decomposition) and environmental control (such as NOx-SCR, CO removal). He authored and coauthored [more than 300 publications](http://www.taozhang.dicp.ac.cn/english/Publications/publications1501.php) in peer-reviewed scientific journals. He has applied more than 140 patents and 57 of them were licensed. Prof. Zhang is an associate editor-in-chief of Chinese Journal of Catalysis (since 2007) and is serving on the advisory boards of Applied Catalysis B (since 2008), ChemPhysChem (since 2010), Chemical Propellants & Polymeric Materials (since 2006). He has served as a Guest Editor of special issues for CHEMSUSCHEM (one time) and Energy Env. Sci. (one time). Dr. Zhang has also received several research awards, including the Distinguished Award of Chinese Academy of Sciences (2010), Zhou Guang Zhao Foundation Award for Applied Science (2009), Excellent Young Scientist Award of Chinese Catalysis Society (2008), National Award of Technology Invention (Second Grade, 2008, 2006, 2005).

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Prof. Can Li received his PhD degree in 1988 from Dalian Institute of Chemical Physics. He worked as post-doc fellow and visiting professor at Northwestern University (USA), The University of Liverpool (UK), Tokyo Institute of Technology (Japan), Lehigh University(USA) and Université Pierre et Marie Curie, Paris VI (France). He was promoted to a full professor in Dalian Institute of Chemical Physics, 1993, and was elected to a member of the Chinese Academy of Sciences in 2003, a member of the Academy of Sciences for Developing World (TWAS) in 2005, and the fellow of Royal Chemical Society in 2005, the member of Academia Europaea in 2008. He was appointed to the Director of State Key Laboratory of Catalysis in 1998, elected to the chairman of the Catalysis of China in 2005, and the President of the International Association of Catalysis Societies in 2008 respectively. He is on the editor boards of more than 15 academic international and national journals.

Prof. Can Li has published more than 400 peer-reviewed papers with over 5000 citations, granted 30 patents and delivered more 200 oral and seminar presentations at international conferences, universities and research institutions in the world, 60 invited and plenary lectures at national and international conferences. Under his supervision, 60 graduate students have obtained their PhD degrees. Among the prestigious awards he received are the “International Catalysis Award”, Hong Kong “Qiu-Shi Outstanding Young Scientist Award”, “Ho Leung Ho Lee Prize”, and “National Award for Outstanding Young Scientists in China”. Prof. Can Li is the invited professor of Université Pierre et Marie Curie, Paris VI, France and honorary professor of the University of Queensland, Australia.

Prof. Can Li has been studying catalysis and materials at molecular level and making effort to reveal the essential relationship between catalytic performance and the catalyst structure. Prof. Can Li has applied these understandings of the fundamental principles of catalysis to the design and development of more selective and active catalysts for practical applications in energy, fine chemicals and environmental industries. Prof. Can Li’s research area including catalysis, spectroscopy and solar energy.

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Dr. Zhang is now a Professor of Physical Chemistry at Solar Energy Division, Dalian National Laboratory for Clean Energy (DNL). He ever spent about thirteen years in Nankai University to earn his bachelor, Ph. D. degree (in 2004) and work as a staff. He visited the University of Pierre & Marrie Curie and worked with Dr. Juliette Blanchard and Dr. Xavier Carrier. After one year’s stay, he moved to Prof. Kazunari Domen’s laboratory at the University of Tokyo, working as a postdoc researcher and an assistant professor separately. To date, he has published more than 50 SCI/EI papers in some peer-reviewed journals such as *Nat. Commun., J. Am. Chem. Soc.* and *Chem. Commun.* etc. with total cited times of over 700.

Zhang’s research interest was focus on development of novel nano-materials and porous materials for some reactions related to environmental and energy catalysis. His current research object is to achieve photocatalytic overall water splitting for hydrogen production using materials with wide visible light absorption together with the following topics: i) novel synthesis of wide visible light-responsive semiconductors with controllable electronic, crystalline and surface structures; ii) development of cocatalysts for efficient water splitting; iii) fabrication of heterogeneous interface for efficient charge transfer; iv) understanding mechanism of solar water splitting; v) comprehensive configuration of catalytic systems with high quantum efficiency of water splitting.

**Solar Hydrogen Production from Water by Heterogeneous Photocatalysis**

Fuxiang Zhang

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Solar energy supply is inexhaustible in human terms, and its use is harmless to our environment and climate.[1] Scientists around the world are working towards the goal of developing technologies to harness energy from the sun to produce fuels. Solar hydrogen production using a powder photocatalyst is a potentially clean and renewable artificial photosynthesis solution to convert solar energy into hydrogen fuel.[2] In the past decades, increasing interests in this field have been paid to developing materials to capture and channel sunlight; deepening understanding of photosynthesis; and discovering new catalysts to make the chemistry possible. In this talk, I will present the recent results on solar hydrogen production in the Solar Energy Division, Dalian National Laboratory for Clean Energy (DNL). It involves photocatalyst materials, cocatalysts as well as their interface etc.. Meanwhile, the feasibility in promoting photogenerated charge separation and consequently fabricating efficient solar-chemical conversion systems by crystal engineering, hetero-phase junction or dual cocatalysts etc. will be discussed.

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Dr. Aiqin Wang joined Prof. Tao Zhang’s group after she received PhD degree in 2001 from Dalian Institute of Chemical Physics (DICP). In 2003, she moved to National Taiwan University as a postdoctoral fellow in Prof. Chung-Yuan Mou’s group for synthesis and catalysis of gold-based alloy nanoparticles until 2005. Then, she went back to DICP and joined Prof. Tao Zhang’s group where she was promoted to a full professor in 2009. Her current research interests involve catalysis by nano gold and gold alloy particles, catalytic conversion of biomass, and design and synthesis of new catalytic materials. She has published more than 120 peer-reviewed papers in high-level journals.

**Catalytic Transformation of Biomass to Ethylene Glycol**

Aiqin Wang,Tao Zhang\*

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Declining fossil fuel reserves and the global climate change associated with the consumption of fossil fuel have triggered intensive interest in developing renewable energy sources. Biomass is the only renewable organic carbon source in nature, which endows it with unique advantages in producing various industrially important chemicals. Cellulose is the most abundant biomass on earth, and the rich hydroxyl groups in the molecules make it an ideal feedstock for the production of polyols. However, the intra- and inter-molecular hydrogen bonding network protects the glycosidic bonds from attack by most solvents or catalysts, and the degradation of cellulose under milder conditions has therefore become a challenging task. In this presentation, we show that under the catalysis of multi-functional tungsten-based catalysts, cellulose could be transformed into ethylene glycol with a high conversion and selectivity.[1-10] The performances of various catalyst formulations containing tungsten compounds were discussed, and the reaction mechanism was proposed based on the characterizations of the catalysts and the reaction kinetics.

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Prof. Xiulian Pan works in the field of nanocatalysis at the State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics (DICP). Her current research interests center around nano-structured carbon for catalysis, including carbon nanotubes, graphene and ordered mesoporous carbon, as well as C-SiC based composites. These materials are either used directly as catalysts or supports for metal components. Therefore, the studies involve synthesis and functionalization (including heteroatom doping) of nano-structured carbon. Particular attention is paid to the fundamental understanding of the confinement effects within limited space on catalysis and utilization of these effects for the activation and conversion of CO, CO2 and N2.

**Confined Catalysis within Carbon Nanotubes**

Xiulian Pan

*State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics,*

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An increasing numbers of studies demonstrate that confinement of metal nanoparticles inside CNTs as catalysts often significantly enhance their activities. [1-3] CO hydrogenation, CO oxidation, ammonia decomposition, selective hydrogenation and oxidation of hydrocarbons, and electrocatalytic reduction of carbon dioxide are just some examples among the list. The confinement effects can be understood from two aspects: the metal catalysts, and reactant molecules (as well as intermediates and products). Examples will be particularly given for the modification on the physiochemical properties of metal catalysts and the carbon layer due to the host-guest interaction. Thus, the adsorption and activation of reactant molecules, stabilization of specific intermediates or products through interactions can be changed. This could have a profound effect on reaction equilibria and rates, and may also alter completely the reaction mechanisms.

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Prof. Shen got his PhD degree from the Institute of Coal Chemistry, Chinese Academy of Sciences in 1995. He then conducted postdoc research in Korean and Japan during 1996-2001. In 2001, he joined the State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences.

The research activities of Prof. Shen`s group are mainly concentrated on two aspects. One is the synthesis and assembly of catalytic materials with controlled particle size and morphology in nano-scales, involving both metal and metal oxides. Another target is to use these catalytic materials for chemical reactions that are potentially significant for energy conversion and environmental protection, such as conversion of methanol, DME and ethanol, selective oxidation of light oxygenates, transformation of biomass-derived compounds and environmental processes. The aim is to integrate the two aspects for establishing the structure-reactivity relationship which is the core of heterogeneous catalysis.

**Morphology-dependent Nanocatalysis: Rod-shaped Oxides**

Wenjie Shen

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Nanostructured oxides are widely used in heterogeneous catalysis where their catalytic properties are closely linked with the size and morphology at nanometer level. The effect of particle size has been well decumented in the past decades, but the shape of the catalyst nanoparticles has rarely been addressed. Here we illustrate that the redox and acidic-basic properties of oxides are largely dependent on their shapes by taking Co3O4, Fe2O3, CeO2 and La2O3 nanorods as typical examples. The catalytic activities of these rod-shaped oxides are mainly governed by the chemical nature of the exposed crystal planes. For instance, the predominant presence of {110} planes which are rich in active Co3+ on Co3O4 nanorods resulted in a much higher activity for CO oxidation than the nanoparticles that mainly exposed the {111} planes. The simultaneous exposure of iron and oxygen ions on the {110} surfaces of Fe2O3 nanorods has significantly enhanced the adsorption and activation of NO and ammnia and consequently promoted the efficiency of DeNOx process.

Moreover, the exposed facets of these rod-shaped oxides mediated the reaction performance of the integrated metal-oxide catalysts. Au/CeO2 catalysts exhibited outstanding stability under water-gas shift conditions owing to the strong bonding of gold particle on the rod-shaped CeO2 support where the formed gold-ceria interface was resistant towards sintering. Cu nanoparticles dispersed on La2O2CO3 nanorods efficiently catalyzed dehydrogenation of primary aliphatic alcohols based on the uniue role of the exposed {110} planes on the oxide support. Morphology control at nanometer level allows preferential exposure of the catalytically active sites, providing a new stragegy for the design of highly efficient nanostructured catalysts.

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**“Oxide-on-Metal” Inverse Catalysts for Low Temperature Oxidation Reactions: from Model Systems to Supported Nanocatalysts**

Qiang Fu

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Heterogeneous catalysts, often consisting of metal nanoparticles (NPs) supported on high-surface-area oxide solids, are widely used in industrial chemical reactions. The importance of oxides in heterogeneous catalysts has been increasingly recognized that they are not just a support to help the dispersion of supported metal NPs. Moreover, they can affect the catalytic process through the interaction with supported metal NPs. In the case of reducible transition metal oxides (TMOs), such interaction can become so prominent that the metal-oxide interface is often considered to play a key role in catalytic reactions. Here, we show that, oxides covering metal surface so-called “inverse catalysts”, when controlled in a proper way, can be utilized to enhance the catalytic performance. Highly dispersed TMO nanostructures may be deliberately constructed on the surface of NMs, forming oxide-on-metal inverse catalysts. The surface TMO phases are often metastable and two-dimensional (2D), owing to the strong interaction between TM cations and NM atoms underneath [3]. TM atoms at the periphery sites of the 2D TMO nanostructures are coordinatively unsaturated, which exhibit extraordinary reactivity and stability in their interaction with reactants. Therefore, the TMO-NM interfaces exert a unique chemical environment to confine the active metal centers, which are not in their thermodynamically stable state but can be kinetically trapped at the interface and in certain reaction environments.

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Zhitao Xiong is a professor of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences (DICP, CAS). He received his BSc, MSc and PhD degree in 1993, 1996 and 1999, respectively, from Xiamen University. He started his research on hydrogen storage in 2000 when he was a research fellow in the Department of Physics, National University of Singapore. He joined DICP in 2008 under the Hundred Talent Project. His current research focuses on the synthesis and application of high capacity hydrogen storage materials.

**Investigations on B-N Based Hydrogen Storage Materials**

Zhitao Xiong

*Dalian Institute of Chemical Physics*

Safe and high efficient hydrogen storage is one of the prerequisite technologies for the coming “hydrogen economy”. In the past decades, several novel material systems including analate, borohydride, amide-hydride combination, ammonia borane (NH3BH3) and derivatives were developed for practical hydrogen storage, among which ammonia borane possesses the highest hydrogen content (19.6 wt%) and therefore received the most attentions. Thermolysis of NH3BH3 encounters the problems of high kinetic barrier, poisonous side product, irreversibility and sample foaming and tremendous efforts have been devoted to improve the desorption kinetics of this chemical hydride by using a variety of catalysts and supporters. However, to enable reversible hydrogen storage composition of NH3BH3 needs to be changed to tune its thermodynamics. In this effort, alkali and alkaline earth metal hydride, imide and amide were employed to interact with NH3BH3 to form amidoborane and amidoborane ammoniate. Presence of dihydrogen bonding network helps to stabilize all these new structures and, even more importantly, the increase of stability of hydride reactant, together with a decrease of B-N bond strength in the dehydrogenation product, leads to reaction enthalpy changing from exothermic to endothermic. Generally, an endothermic dehydrogenation reaction is applicable for reversible hydrogen storage.

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Wei-Xue Li is a Professor of Physics Chemistry and Group Leader of Theoretical Catalysis at Dalian Institute of Chemical Physics (CAS) since 2004. He defended the Ph. D. degree at Institute of Mechanics, CAS (1998), and as a post-doctoral researcher spent five and half years (1999-2004) at Fritz-Haber-Institute (MPG) and Aarhus University (Denmark). Wei-Xue Li serves as a member of the editorial boards of Surface Science, and Head of Max-Planck-Society and Chinese Academy of Science Partner Group for “First-Principles High-Pressure Oxidation Theory”. He was awarded the National Natural Science Foundation of China for Distinguished Young Scholar (2012), CAS “Hundred Talents” (2004). His scientific career builds on the development of theoretical and computational approaches to tackling the heterogeneous catalysis. He has contributed over 70 high-quality journal publications. Professor Li’s research focuses on the development of kinetic theory of sintering of supported metal particles and ab initio thermodynamics method. Density functional theory calculations have been applied to various catalytic reactions including syngas conversion and Fischer-Tropsch synthesis, methanol reforming and CO oxidation over metal, metal oxide and metal carbide etc.

Representative Publications

1. Atomistic Theory of Ostwald Ripening and Disintegration of Supported Metal Particles under Reaction Conditions; R. H. Ouyang, J. X. Liu, W. X. Li\*; *J. Am. Chem. Soc.* 135 (2013) 1760-1771
2. Platinum-modulated Cobalt NanoCatalysts for Low Temperature Aqueous Phase Fischer-Tropsch Synthesis; H. Wang, W. Zhou, J. X. Liu, R. Si, M. Q. Zhong, H. Y. Su, J. A. Rodriguez, S. J. Pennycook, J. C. Idrobo, W. X. Li\*, Y. Kou\*, and D. Ma\*; *J. Am. Chem. Soc*. (2013) DOI:10.1021/ja400771a
3. Carbon Chain Growth via Formyl Insertion on Rh and Co Catalysts in Syngas Conversion; Y. H. Zhao, K. J. Sun, X. F. Ma, J. X. Liu, D. P. Sun, H. Y. Su, W. X. Li*\*;* *Angew. Chem. Int. Ed.*50 (2011) 5335-5339
4. In-situ Oxidation Study of Pt(110) and its Interaction with CO; D. R. Butcher, M. E. Grass, Z. H. Zeng, F. Aksoy, H. Bluhm, W. X. Li\*, B. S. Mun\*, G. A. Somorjai, Z. Liu\*; *J. Am. Chem. Soc.* 133 (2011) 20319-20326
5. Interface-Confined Ferrous Centers for Catalytic Oxidation, Q. Fu, W. X. Li, Y. Yao, H. Liu, H. Y. Su, D. Ma, X. K. Gu, L. Chen, Z. Wang, B. Wang, X. H. Bao\*; Science 328 (2010) 1141-1144

**Kinetic Theory of Ostwald Ripening of Supported Metal Particles under Reaction Conditions**

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Understanding Ostwald ripening and disintegration of supported metal particles under operating conditions has been of central importance in the study of sintering and dispersion of heterogeneous catalysts for long term industrial implementation. To achieve a quantitative description of these complicated processes, an atomistic and general theory taking into account of the reaction environment, particle size and morphology, and metal-support interaction is developed. It includes energetics of supported metal particles, formation and diffusion of monomers on supports, and corresponding sintering rate equations, in the presence of reactants at arbitrary temperature and pressure. The thermodynamic criteria for the reactant assisted Ostwald ripening and induced disintegration are formulated, and the influence of reactants on sintering kinetics and redispersion are mapped out. Most data required in the theory can be calculated by first-principles theory, a fact that allows for the rapid exploration of sintering and disintegration of supported metal particles in huge phase space of structures and compositions under various reaction environments. The theory is applied to oxide supported Rh and Au particles in the presence of carbon monoxide, and rationalizes the broad temperature, pressure, and particle size range over which the sintering and redispersion occurred in such experiments. General strategies of suppressing the sintering of the supported metal particles and facilitating the redispersions of the low surface area catalysts are proposed in the end.

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